Trichloroethylene
79-01-6 | DTXSID0021383

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 97.2 °C

Global applicability domain: Inside

Local applicability domain index: 6.50e-01

Confidence level: 7.46e-01

Nearest Neighbors from the Training Set

Image not found
Trichloroethylene
Measured: 87.2
Predicted: 97.2

Image not found
Thiophene, 2,3-dihydro-
Measured: 112
Predicted: 112

Image not found
Thiophene, 2,5-dihydro-
Measured: 122
Predicted: 115

Image not found
Epibromohydrin
Measured: 135
Predicted: 128